



Mathematical Modelling and Simulation of Fluidized Bed Reactor for Hydrogen Production from Bioethanol

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ABSTRACT

Mathematical models describing the steady state behaviour of fluidized bed reactor for hydrogen production from bioethanol via steam reforming process have been developed in this work. The models were developed by the application of the principles of conservation of mass and energy incorporating the two-phase principle of fluidization. The kinetic model for the bioethanol steam reforming process was developed from first principle by applying the Eley-Rideal mechanistic approach. The hydrodynamic models were obtained from literature and together with the kinetic model were incorporated into the developed mathematical models. The developed models consist of systems of non-linear Ordinary Differential Equations (ODEs) and MATLAB programming language was used to solve the system of equations simultaneously. Model predictions for C_2H_6O , H_2O , CO_2 and H_2 showed excellent agreement with deviations of 10.7%, 3.89%, 7.69% and 9.0% respectively from pilot plant data at same prevailing conditions. Sensitivity analysis performed on the reactor showed optimum possible values for superficial velocity of 0.25m/s and bubble diameter of 0.075m.

Keywords: Modelling and Simulation, Fluidized Bed Reactor, Steam Reforming, MATLAB

1. INTRODUCTION

The recent concerns about the continuous decline in the availability and affordability of domestic reserves of petroleum and natural gas fuels, coupled with the increasing reliability problems in the geopolitics of world's energy supply, global warming and climate change have led to a renewed interest in the use of renewable energy and materials instead of fossil fuels. The demand for energy is rising due to exponential increase in population and economic development and there is need for energy supply to meet up with the daily needs in today's society. However, the over dependency on fossil fuel to meet up with the growing demand has resulted in a continuous decline of petroleum and natural gas reserves and negative environmental impacts caused by emissions generated from the combustion process of the fossil fuels (Akande *et al.*, 2006). The search for an alternative renewable and less polluting energy sources has gained prominence because of the environmental issues and increasing energy demand associated with fossil fuel. Of all the various energy sources and energy carriers under study, hydrogen has been identified as the best alternative source of energy that could easily replace petroleum-based fuels (fossil fuel) as the byproducts of its combustion with oxygen are only water and energy (Bineli, 2016).

Hydrogen is the most abundant chemical elements in the world, comprising almost three-quarters of the universe's entire mass (Marino, *et al.*, 2001). Although abundant, hydrogen is often found combined with other elements in the natural environment and a series of different processes are required to isolate it. The main methods of producing hydrogen employ fossil fuels, water and biological processes. However, hydrogen production from fossil fuels by steam reforming, or from water by electrolysis and thermochemical decomposition, is not environmentally friendly and is expensive (Amorim *et al.*, 2009). The methods employed for the production of hydrogen are mainly from natural gas using the process of reforming which leads to environmental problems. Among the different raw materials available, alcohols are very promising raw material because they are easily

disintegrated in the presence of water to produce hydrogen-rich mixture. Steam reforming of methanol has been studied extensively in recent years, (Ahmed & Krumpelt, 2001) investigated its possible use as an alternative raw material for energy production but have a major drawback, which is its high toxicity. Among the various processes proposed, steam reforming of bioethanol for the production of hydrogen proves to be very attractive because bioethanol can be produced by simple fermentation of renewable resources like biomass, it is easy to transport, biodegradable, contains high hydrogen content, easy to store and more importantly it is nontoxic (Nicu, *et al.*, 2017). More significantly, bioethanol is carbon (CO₂) neutral since the amount of CO₂ produced by steam reforming is consumed by the biomass growth, and this offers a nearly closed carbon loop and does not contribute to greenhouse gas emissions. Steam reforming of bioethanol occurs at relatively lower temperatures compared with fossil fuels, and has been widely studied due to the high yield of hydrogen from the process. Additionally, bioethanol is economically, environmentally and strategically promising as an energy source. Bioethanol can be a renewable hydrogen source because virtually any biomass can now be converted into bioethanol as a result of recent advances in biotechnology (Abdulwahab & Saidat, 2013). Hydrogen obtained from reforming of bioethanol is a very good energy vector especially in fuel cells technology applications for the production of electricity (Men, 2008). Hydrogen production from bioethanol has numerous advantages compared to other hydrogen production methods, including steam reforming of methanol and hydrocarbons. Unlike hydrocarbons, bioethanol is easier to reform and is sulphur free, which is a catalyst poison in the reforming of hydrocarbons. In addition, unlike methanol, which is produced from hydrocarbons and has a relatively high toxicity (Abdulwahab & Saidat, 2013), bioethanol is completely biomass-based and has low toxicity and as such, it provides less risk to the population. The fact that methanol is derived from fossil fuel resources also makes it an unreliable energy source in the long run due to depletion of petroleum reserves. Hydrogen finds useful application in fuel cells for the production of electricity in a very efficient and clean operation, since the only by-product is water and energy. Commercialization of fuel cell technology for electric power generation has been given due attention in recent times because it finds useful applications in electric vehicles and power plants. Kunzru, (2015) predicted that in the near future, hydrogen would be used, largely, as a major energy carrier for the production of electricity for mobile and small-to-medium scale stationary applications. Abayomi, *et al.*, (2006) discussed the situation for a sustainable hydrogen economy in the 21st century and concluded that fuel cells will play a major role in meeting the energy demands of the future. Hence, in order to support this predicted sustainable hydrogen economy, it is key to produce hydrogen cleanly from renewable energy resources.

The consideration of fluidized bed reactor is acceptable due to its numerous positive features (Amorim *et al.*, 2009), such as the accumulation of large amounts of biomass attached to the support medium, high organic loading rates (OLR), low hydraulic retention times (HRT), and good mixing characteristics, which optimize mass and heat transfer between the substrate and microorganisms. In addition, fluidized bed reactor allows high-speed stirring in the liquid phase, which favours hydrogen release at this stage. Mathematical modelling helps us to qualitatively and quantitatively dichotomize real life problems in order to assess the significance of their various parts, which can lead to the original motivating problem becoming a building block for the understanding of more complex systems. Good models provide the flexibility to be developed systematically allowing more accurate answers to be obtained by solving extensions of the model's mathematical equations. This work is intended to be a contribution to the state of mathematical modelling and simulation of fluidized bed reactors for hydrogen production from bioethanol. Fossil fuels constitute the greater part of our daily energy consumption, greenhouse gas emissions released during their combustion, amass in the atmosphere and lead to an increase of global temperatures. The resulting change of climate is detrimental to life on earth and it is negatively affecting our environment. In addition, the continuous decline in the availability and affordability of hydrocarbons reserves, and the need for hydrogen to be utilized as a major energy source for fuel cell technology, necessitated this research. This research applies the principles of chemical engineering in the development of mathematical models of fluidized bed reactor to study the production of hydrogen which is a reliable energy carrier obtained from bioethanol; a renewable and nontoxic raw material.

2. Materials and Methods

2.1 Development of Models

Modelling is a systematic mathematical approach to formulation, simplification and understanding of behaviours and trends in real life problems. Mathematical models also allow for the exploration of conjectures and hypothetical situations that cannot normally be de-coupled or for parameter ranges that might not be easily accessible experimentally or computationally (Thomas & Mark, 2015). Steam reforming of bioethanol in a fluidized bed reactor involves chemical reactions as well as mass transport, which are profoundly affected by hydrodynamics in the reactor (Amorim *et al.*, 2009). Figure 1 shows a hypothetical representation of a two phase fluidized bed reactor comprising the emulsion phase and bubble phases. The emulsion phase consists of the catalyst particles and the steam flow rate is equivalent to the minimum fluidization velocity.

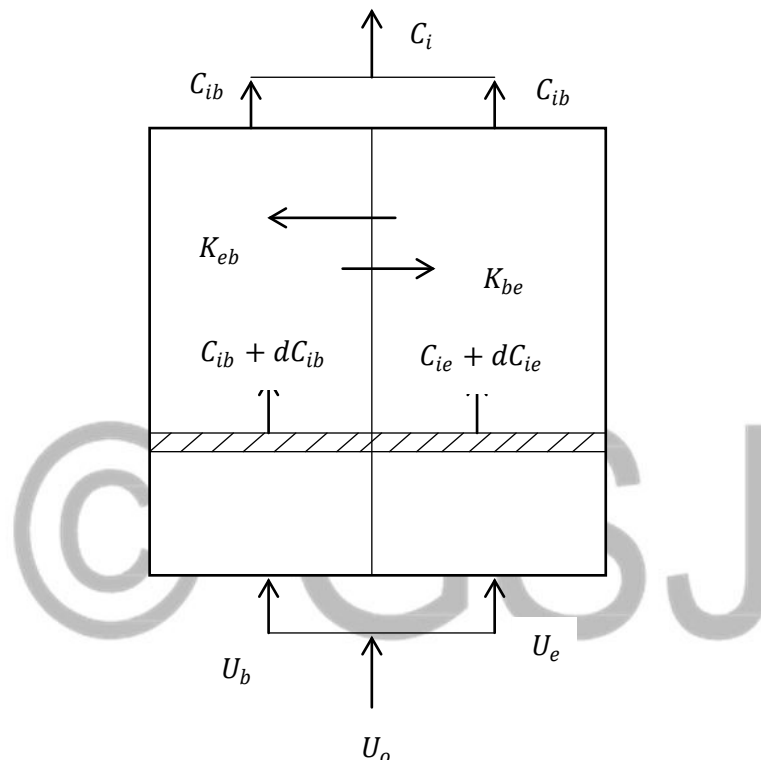


Figure 1: Hypothetical Representation Two Phase Fluidized Bed Reactor for Steam Reforming of Bioethanol

2.1.1 Model Assumptions

Assumptions are aimed at simplifying the model but not limiting it to be a true representation of the system been considered.

- i. The fluidized bed consists of two phases,' namely, bubble and emulsion phases, which are homogeneously distributed statistically.
- ii. The flow of gas in excess of the minimum fluidization velocity passes through the bed in the form of bubbles.
- iii. The feed enters the bed at incipient velocity and is partitioned between the emulsion phase, here the velocity is that of minimum fluidization and the bubble phase where the velocity is $U_o - U_{mf}$
- iv. The bed is characterized by an equivalent bubble size, and the flow of gas in the bubbles is in plug flow.
- v. The emulsion phase can be considered to be either totally mixed or plug flow system, but since axial diffusion (transport by effective diffusion) in the emulsion is negligible, the reacting emulsion phase is considered to be in plug flow and non-isothermal.

- vi. The bubble phase is particle free and moves upward as plug flow with negligible catalytic reaction occurring.
- vii. The products consumptions are not expected to be hindered by diffusion, hence, the effectiveness factor is assumed to be equal to unity.

2.1.2 Material Balance Equation

(a) Bubble phase: Application of the law of conservation of mass to gases in the bubble-phase, with the assumptions of no accumulation and without reforming reactions, gives the material balance on species i over an elemental volume of $A_b \Delta h$ as:

$$\frac{\partial C_{ib}}{\partial t} = -U_b \frac{\partial C_{ib}}{\partial h} + D_{ib} \frac{\partial^2 C_{ib}}{\partial h^2} - K_{be}(C_{ib} - C_{ie}) \quad (1)$$

Expressing equation (1) in dimensionless form and assuming steady state yields

$$0 = -\frac{U_b \partial y_{ib}}{H \partial Z} + \frac{D_{ib} \partial^2 y_{ib}}{H^2 \partial Z^2} - K_{be}(y_{ib} - y_{ie}) \quad (2)$$

Since dispersion causes a decrease in the overall yield of the process, neglecting the dispersion term $\frac{D_{ib} \partial^2 y_{ib}}{H^2 \partial Z^2}$, the resulting equation takes the form of a plug flow as;

$$\frac{dy_{ib}}{dZ} = -\frac{HK_{be}}{U_b}(y_{ib} - y_{ie}) \quad (3)$$

Equation (3) represents the bubble phase model.

(b) For the Emulsion phase

Application of the law of conservation of mass with steam reforming reactions in the emulsion-phase on species i over an elemental volume of $A_b \Delta h$ based on the above assumptions gives

$$\frac{\partial C_{ie}}{\partial t} = -\frac{U_e \partial C_{ie}}{\varepsilon_{mf} \partial h} + \frac{D_{ie} \partial^2 C_{ie}}{\varepsilon_{mf} \partial h^2} + \frac{A_b K_{be}}{A_e \varepsilon_{mf}}(C_{ib} - C_{ie}) + \frac{R_{ie}}{\varepsilon_{mf}} \quad (4)$$

Writing the model in dimensionless form and assuming steady state condition we have;

$$\frac{dy_{ie}}{dZ} = \frac{HA_b K_{be}}{A_e U_e}(y_{ib} - y_{ie}) + \frac{HR_{ie}}{C_e U_e} \quad (5)$$

Equation (5) represents the model for the emulsion phase.

2.1.3 Energy Balance Models

2.1.3.1 Energy Balance for the Bubble Phase

The energy balance equation, based on the principle of chemical engineering for heat evaluation of processes and systems, will be applied to the bubble phase to study the temperature behaviour of the phase. Applying the law of conservation of energy to a differential element of the bubble phase noting the bubble phase is modelled as plug flow, we have:

$$v_{ob} \rho_{ib} C_{p_{ib}} T_b = v_{ob} \rho_{ib} C_{p_{ib}} (T_b + dT_b) + J_{be} \rho_{ib} C_{p_{ib}} (T_b + T_e) dV_{ib} \quad (6)$$

Simplification of equation (6) gives;

$$\frac{dT_b}{dh} = \frac{A_b J_{be} (1-\varepsilon)(T_b - T_e)}{v_{ob}} \quad (7)$$

Expressing equation (7) in dimensionless form yields:

$$\frac{dT_b^I}{dz} = \frac{J_{be} (1-\varepsilon)(T_b^I - T_e^I)H}{U_b} \quad (8)$$

where: v_{ob} is the volumetric flow rate of species i in the bubble phase, ρ_{ib} is the density of species i in the bubble phase, $C_{p_{ib}}$ is the specific heat capacity of species i in the bubble phase, T_b and T_e are the temperature in the bubble and emulsion phases respectively, $(-r_{ib})$ is the rate of reaction of species i in the bubble phase, (ΔH_{rib}) is the heat of reaction of the respective species i , V_{ib} is the volume of species i in the bubble phase, J_{be} is the bubble to emulsion phase heat transfer coefficient, t is the time spent in the bubble phase, T_b^I is the dimensionless Temperature in the bubble phase, T_e^I is the dimensionless Temperature in the emulsion phase, U_b is the velocity of gas in the bubble phase, J_{be} is the gas interchange coefficient between the bubble and emulsion phases based on the volume of bubbles, H is the height of the bed, z is the dimensionless height.

2.1.3.2 Energy Balance in the Emulsion Phase

The emulsion phase is made up of the catalyst particles alongside steam, which is the gasifying agent. Hence, the energy balance in the emulsion phase will incorporate the characteristic features of the catalyst and steam for better representation of the temperature variation in the phase. Applying the principle of conservation of energy for the emulsion phase gives:

$$-\frac{dT}{dh} = \frac{\sum_{i=1}^n (\Delta H_R)(-r_i) \rho_s \varepsilon A_R}{(\rho_s v_{os} C_{p_s} + \rho_{cat} v_{cat} C_{p_{cat}})} \quad (9)$$

Expressing equation (9) in dimensionless form:

$$-\frac{dT_R}{dZ} = \frac{\sum_{i=1}^n (\Delta H_R)(-r_i) \rho_s \varepsilon A_R H_R}{(\dot{m}_s C_{p_s} + \dot{m}_{cat} C_{p_{cat}}) T_{ref}} \quad (10)$$

Equation (10) represents the energy balance for the Emulsion phase.

where: C_{p_s} is the specific heat capacity of steam at constant pressure; $C_{p_{cat}}$ is the specific heat capacity of the catalyst; ρ_{cat} is the density of the catalyst; v_{cat} is the volumetric flowrate of the catalyst; ρ_s is the density of steam; ΔH_R is the heat of reaction; T is the inlet temperature; dT is the temperature change within differential element; ε is the void fraction; T_R is the dimensionless temperature; T_{ref} is the reference temperature; Z is the dimensionless height; H_R is the height of reactor

2.2 Hydrodynamic Relationships

Functional relationships among the parameters and variables that depend on the hydrodynamics of the fluid-bed are given as follows:

(a) Bubble and Emulsion Phase Velocities

The bubble phase velocity U_b can be estimated using the formula (Kunii and Levenspiel, 1991):

$$U_b = U_o - U_{mf} + U_{br} \quad (11)$$

where U_{br} represents the rise velocity of a single bubble in the bed and is given by

$$U_{br} = 0.711 (gd_b)^{\frac{1}{2}}$$

where, d_b represents the bubble diameter

The emulsion phase velocity $U_e = U_{mf}$

where U_{mf} is the minimum fluidization velocity

(b) Interchange Transfer Coefficient

This is estimated using Kunii and Levenspiel (2001) correlation;

Bubble – Emulsion Transport Coefficient (K_{be})

K_{be} is obtained by the addition of the two parallel resistances.

$$\frac{1}{K_{be}} = \frac{1}{K_{bc}} + \frac{1}{K_{ce}} \text{ i.e } K_{be} = \frac{K_{bc} \cdot K_{ce}}{K_{bc} + K_{ce}} \quad (12)$$

Bubble Diameter

The bubble diameter d_b is estimated using Mori and Wen (1975) correlation;

$$d_b = D_{bm} - (D_{bm} - D_{bo}) \exp\left(-0.3 \frac{x}{D}\right)^1 \quad (13)$$

$$D_{bm} = 0.652 \{A(U_o - U_{mf})\}^{0.4} \quad (14)$$

$$D_{bo} = 0.00376(U_o - U_{mf})^2 \quad (15)$$

where D_{bo} is the initial bubble diameter and D_{bm} is the maximum bubble diameter.

The equivalent bubble diameter (Kunii and Levenspiel, 1969) is calculated at the middle of the total bed height, $h = \frac{H}{2}$ (16)

2.3 Kinetic Model

The simulation, design and modelling of any reactor needs information on both the thermodynamic and kinetic properties of the reaction of interest. Mechanistic description based on Eley Rideal assumptions of the bioethanol steam reforming process together with careful kinetic expressions were used in the derivation of the rate equation.

Bioethanol steam reforming reaction is represented by equation (17)

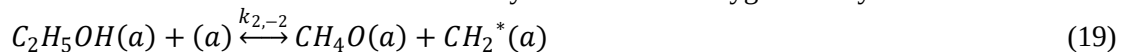


The three steps process for heterogeneous catalysis is given as:

- i. Adsorption of the bioethanol on an active site of the catalyst:



- ii. Dissociation of adsorbed bioethanol into hydrocarbon and oxygenated hydrocarbon fractions:



- iii. Surface reaction of adsorbed oxygenated hydrocarbon fraction with non-adsorbed water vapour:



- iv. Surface reaction of adsorbed hydrocarbon fraction with non-adsorbed water vapour:



where: (a) represents an active site

Let

$C_2H_5OH = A$, $CH_4O(a) = A^*$, $H_2O = B$, $CH_2^* = n^*$, $CO_2 = C$, $C_2H_5OH(a) = A(a)$ and $H_2 = D$

Rate of reaction for each of the reactions (21) – (24) respectively;

$$r_A = -k_1 C_A C_{(a)} + k_{-1} C_{A(a)} \quad (22)$$

$$r_A = -k_2 C_{A(a)} C_{(a)} + k_{-2} C_{A^*(a)} C_{n^*(a)} \quad (23)$$

$$r_A = -k_3 C_{A^*(a)} C_B + k_{-3} C_C C_D^3 C_{(a)} \quad (24)$$

$$r_A = -k_4 C_{n^*(a)} C_B^2 + k_{-4} C_C C_D^3 C_{(a)} \quad (25)$$

Developing the equilibrium relations for each of the rate of reactions (22) – (25) and simplifying we obtain:

$$r_A = \frac{k_o e^{\frac{-E}{RT}} \left[y_A \frac{y_C^2 y_D^6}{K_p y_B^3} \right]}{\left[1 + \left(\frac{k_F y_C y_D^3}{y_B} \right) + \left(\frac{k_G y_C y_D^3}{y_B^2} \right) + \left(\frac{k_E y_C^2 y_D^6}{y_B^3} \right) \right]} \quad (26)$$

$$r_A = \frac{k_o e^{\frac{-E}{RT}} \left[y_A - (y_C^2 y_D^6 / k_p y_B^3) \right]}{\left[(1 + k_A y_A + \left(\frac{k_F y_C y_D^3}{y_B} \right) + \left(\frac{k_G y_C y_D^3}{y_B^2} \right)) \right]^2} \quad (27)$$

$$r_A = \frac{k_o e^{\frac{-E}{RT}} \left[\left(\frac{y_A y_B^3}{y_C y_D^3} \right) - (y_C y_D^3 / k_p) \right]}{\left[1 + k_A y_A + \left(\frac{k_Q y_A y_B^2}{y_C y_D^3} \right) + \left(\frac{k_G y_C y_D^3}{y_B^2} \right) \right]} \quad (28)$$

$$r_A = \frac{k_o e^{\frac{-E}{RT}} \left[\left(\frac{y_A y_B^3}{y_C y_D^3} \right) - (y_C y_D^3 / k_p) \right]}{\left[1 + k_A y_A + \left(\frac{k_F y_C y_D^3}{y_B} \right) + \left(\frac{k_H y_A y_B^3}{y_C y_D^3} \right) \right]} \quad (29)$$

Abayomi *et al.*, (2006) assumed the dissociation of adsorbed bioethanol as the rate-determining step and when compared with experimental data, showed reasonable agreement, which indicated that, the assumption was justified. Furthermore, considering the experimentally estimated values of the

parameters as well as the values of the equilibrium constant, the rate model based on the assumption of dissociation of adsorbed bioethanol as the rate-determining step reduces to equation (30);

$$r_A = \frac{k_o e^{\frac{-E}{RT}} [y_A]}{[1 + k_A y_A]^2} \quad (30)$$

r_A = rate of bioethanol conversion ($\text{mol m}^{-3} \text{s}^{-1}$), k_o = collision frequency,
E = activation energy (kJ mol^{-1}), R = Universal gas constant, T = absolute temperature (K)

The exit concentration from the bubble and emulsion phases were linked together by using the formula developed by Dagde & Puyate (2012) as:

$$y_i = \beta y_{ib} + (1 - \beta) y_{ie} \quad (31)$$

$i = A, B \text{ and } C \text{ for } C_2H_5OH, CO_2, H_2 \text{ respectively.}$

Writing equation (31) in terms of A, B and C.

$$y_A = \beta y_{Ab} + (1 - \beta) y_{Ae} \quad (32)$$

$$y_B = \beta y_{Bb} + (1 - \beta) y_{Be} \quad (33)$$

$$y_C = \beta y_{Cb} + (1 - \beta) y_{Ce} \quad (34)$$

$$\text{where: } \beta = 1 - \frac{U_{mf}}{U_o} \quad (35)$$

2.4 Operating Parameters

The model equations developed contain certain unknown hydrodynamic and kinetic parameters such as the reaction rate constants for the various reaction paths (K_{ij}), the fluidized bed hydrodynamic parameters, (K_{be}), (U_e), (U_b), (U_{br}), etc. These constants have to be determined before integration of the models.

Table 1: Operating and Hydrodynamic Parameters

Parameters	Values
Superficial gas velocity, U_s	0.25 m/s
Minimum fluidization velocity, U_{mf}	0.12 m/s
Bubble velocity, U_b	0.556 m/s
Frequency factor, k_o	$2.08 * 10^3$
Bubble diameter, d_b	0.0487 m
Activation Energy, E	$4.43 * 10^3 \frac{\text{KJ}}{\text{Kmol}}$
Thermodynamic equilibrium constant, K_A	$3.83 * 10^7$
Mass transfer interchange coefficient	4.92 s^{-1}
Mass transfer interchange coefficient between the bubble and emulsion phase, K_{be}	1.86 s^{-1}
Temperature, T	593K
Catalyst pore volume	$0.0029 \text{ m}^3/\text{g}$

Pore size	14.5nm
Catalyst bulk density	1600kg/ m ³

2.5 Solution Techniques

The developed model equations will be solved using MATLAB R2015a ODE 45 solver from Mathworks by employing the fourth order Runge Kutta algorithm in solving the resultant ordinary differential equations (ODEs).

2.5.1 Initial Conditions

The reactants for this work are bioethanol and water, which formed hydrogen and carbon (iv) oxide as products. The mass fraction of the bioethanol and water at the inlet of the reactor are 0.045 and 0.95 respectively, while the mass fractions of the products at the inlet of the reactor are equal zero. The initial conditions at the inlet of the reactor are stated mathematically as:

$$Z = 0; \quad \left\{ \begin{array}{l} y_{Ab0} = y_{Ae0} = 0.045; y_{Bb0} = y_{Be0} = 0.95 \\ y_{Cb0} = y_{Ce0} = y_{De0} = y_{Db0} = 0 \end{array} \right.$$

3. RESULTS AND DISCUSSION

3.1 Validation of Present Models

Table 2 shows the conversion of C_2H_5OH and the yield of products as predicted by the developed model equations in comparison with data obtained from the experimental work of Abayomi, *et al.*, (2006). The outlet concentrations based on the solution of the numerical models for all species were compared with the corresponding concentrations obtained experimentally by Abayomi, *et al.*, (2006) as shown in Table 2. From the comparison, it is seen that there is excellent agreement between the predicted and experimental results.

Table 2: Model Validation

Component	Experimental Data	Model Prediction Fluidized Bed	%Deviation
C_2H_5OH	0.028	0.025	10.7
H_2O	0.822	0.790	3.89
CO_2	0.039	0.042	7.69
H_2	0.111	0.121	9.0

3.2 Discussion

The results obtained for the yield of products and the conversion of the bioethanol predicted by the fluidized bed models developed; which incorporated the Eley-Rideal kinetic mechanisms for bioethanol-steam reforming process along the dimensionless height of the reactor is shown in Figures 2 and 3. Figures 2 and 3 shows the variation of mass fraction of the reactants and products with dimensionless height. From Figure 2, it is seen that the mass fraction of bioethanol (C_2H_6O) decreases along the dimensionless height while the mass fraction of CO_2 and H_2 increases along the dimensionless height. This behavior is as a result of the kinetics of the steam reforming process of bioethanol as described by the Eley-Rideal mechanisms.

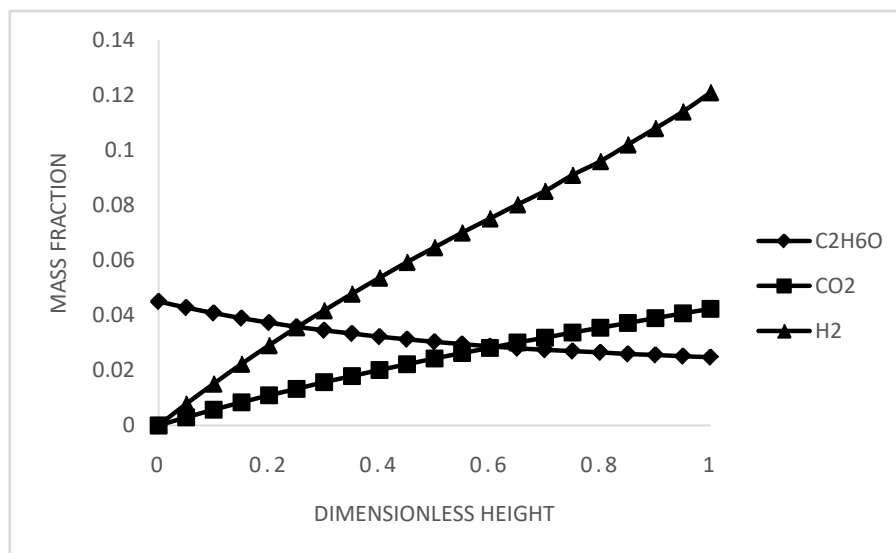


Figure 2: Variation of Mass Fraction with Dimensionless Height

Additionally, the behaviour of the system as shown in Figures 2 and 3 also agrees with the principle of chemical reaction kinetics, which states that the rate of a chemical reaction is directly proportional to the concentration of the reacting species. Indicating a decrease in the concentration of the reacting species in this case (C_2H_6O and H_2O) and an increase in the products CO_2 and H_2 .

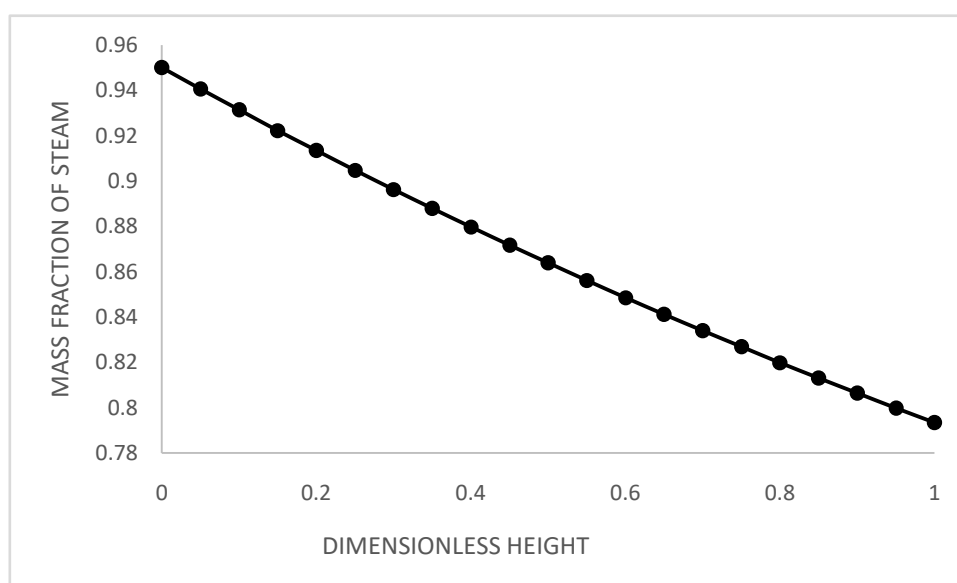


Figure 3: Variation of Mass Fraction of Steam with Dimensionless Height

3.2.1 Variation of Temperature with Dimensionless Height

For any reactor or reaction process, the temperature of reaction is a very important parameter to consider and examine. Reactions are classified based on temperature variation within the reactor as reactions occurs, which further strengthen the importance of temperature in any studies of reactors and reactions. Steam reforming of bioethanol for the production of hydrogen is not an exemption as the effect of reactor temperature is readily noticed due to the nature of reforming reactions. Reforming reactions are mostly endothermic; meaning that there is a decrease in temperature of the reactor as the reaction proceed. The understanding of the variation of temperature is important in both design and modelling of reactors because temperature is a major driving force of most chemical reactions.

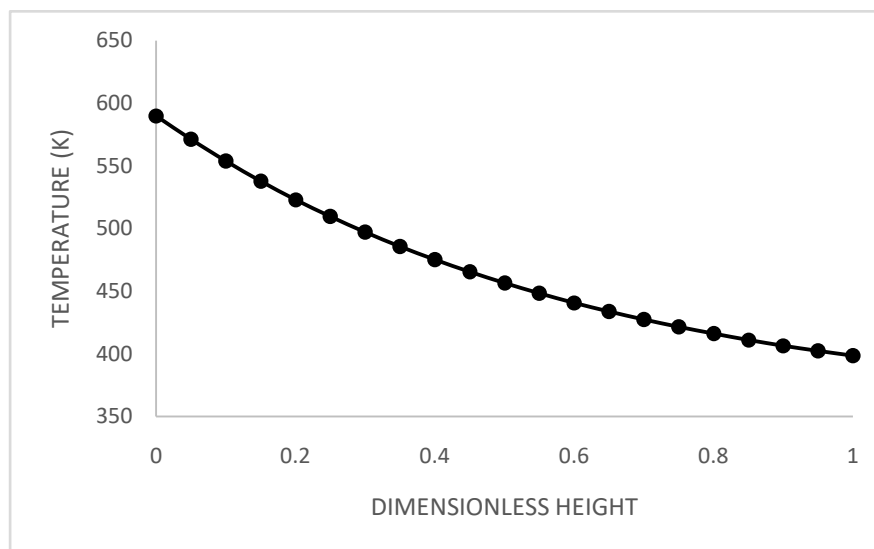


Figure 4: Variation of Temperature with Dimensionless Height

Figure 4 shows the variation of reactor temperature with dimensionless height. From Figure 4, it is seen that the temperature progression along the dimensionless height decreases progressively due to the endothermic nature of steam reforming reaction of C_2H_6O taking place in the reactor. This behavior is in agreement with the research carried out by Abayomi, *et al.*, 2006.

3.2.2 Sensitivity Analysis

Sensitivity analysis is a very important procedure to follow in mathematical modelling of processes and systems. It determines the effect of different functional parameters on the behaviour of the process. Sensitivity analysis is also useful in process optimization and control.

3.2.2.1 Superficial Velocity

The superficial velocity, which is the ratio of the volumetric flow rate and the cross sectional area is a function of the height of the reactor since the cross sectional area of the reactor is a function of the reactor height. Figure 5 shows the variation of the superficial velocity with dimensionless height.

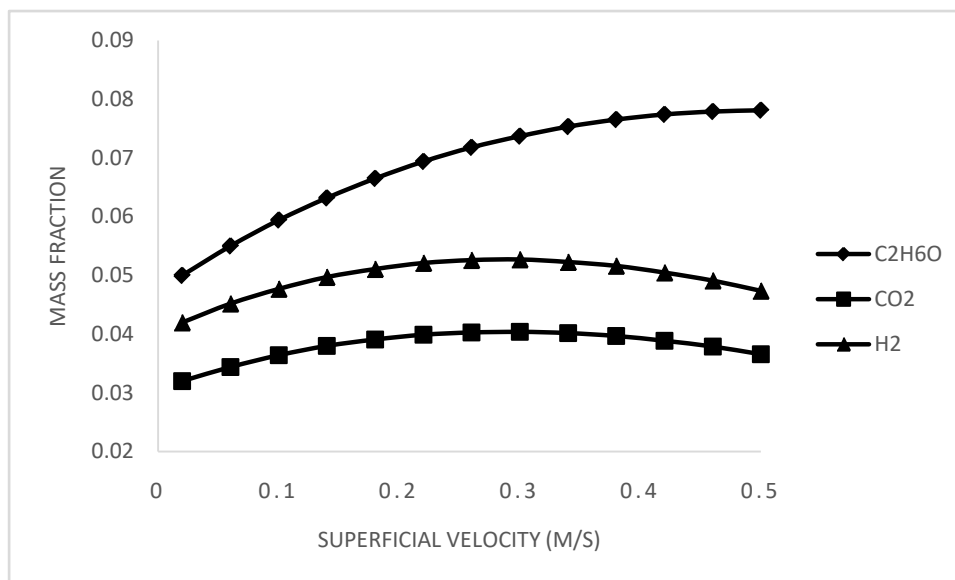


Figure 5: Variation of Mass Fractions with Superficial Velocity

Figure 5 depicts the variation of the mass fractions of the components of the system with superficial velocity. From Figure 5 it is seen that the mass fraction of C_2H_6O increases with an increase in the superficial velocity while the mass fraction of the products CO_2 and H_2 increases slightly and at a point began to decrease with increase in the superficial velocity. The behavior as shown in Figure 5 is a typical for a fluidized bed reactor whenever there is a continuous increase in the superficial velocity. A continuous increase in the superficial velocity of the fluidizing agent results in low residence time for reaction to occur and yield products.

3.2.2.2 Bubble Diameter

This is a very important functional parameter to consider in modelling of fluidized bed reactor because it has a direct influence on the performance of the reactor. The bubble diameter represents the quantity of fluidizing gas above the required for minimum fluidization that moves up along the

centreline of the bed.

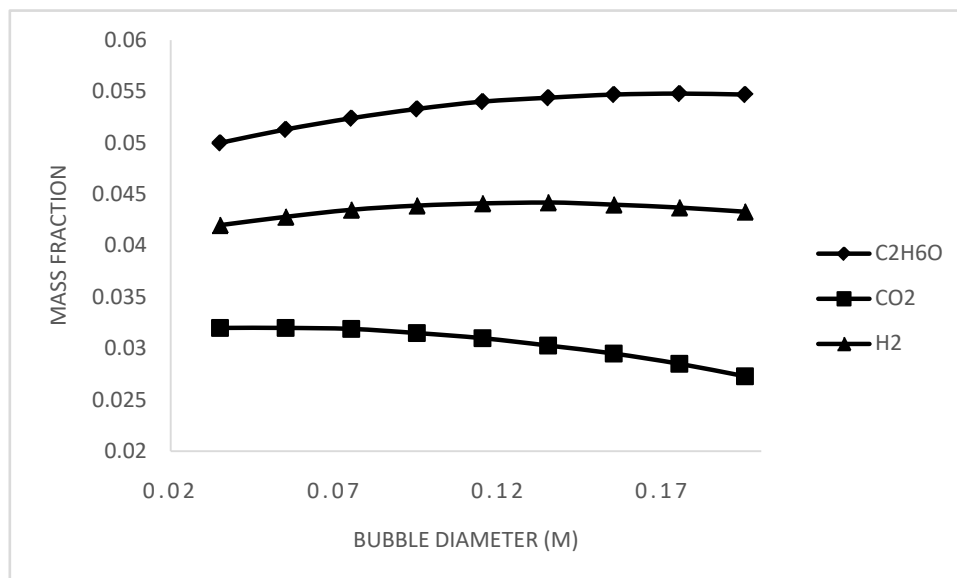


Figure 6: Variation of Mass Fraction with Bubble Diameter

Figure 6 shows the variation of mass fraction of the components of the system with bubble diameter. From Figure 6 it is seen that the mass fraction of CO_2 and H_2 decreases as the bubble diameter increases. In addition, the mass fraction of C_2H_6O increases slightly as the bubble diameter increases. The decrease in the yield of products may be attributed to slugging effect and the fact that an increase in the bubble size causes the bubble to quickly move upward in a plug flow manner and then burst and rains down the particles thereby creating a local space velocity that limits the yield of products.

4. Conclusion

This work entails the development and simulation of detailed but comprehensive mathematical models and computer program that simulates the operation of a fluidized bed reactor for steam reforming of bioethanol for the production of hydrogen. The Eley-Rideal mechanistic approach for heterogeneous reactions as it relates to steam reforming of bioethanol was developed from first principle and incorporated into the models to ensure proper description of the process. The results obtained from the developed mathematical models were compared with experimental results obtained by Abayomi, *et al.*, (2006) and showed excellent agreement.

The following major conclusions can be drawn from this present study;

- The results obtained in this work clearly point to the direct link between the hydrodynamics and reaction kinetics in a fluidized bed reactor.
- The present model has studied the variation of mass fractions of each components with the dimensionless height. The results indicate that as the dimensionless height increases, the yield of products increases in a steady pattern.
- Sensitivity analysis was carried out to study the effect of functional parameters such as the superficial velocity, bubble diameter on the yield of products and temperature variation along the reactor height was considered.
- The vertical one-dimensional differential mass treatment, for the bed, proved to be a reasonable mathematical approach to the simulation.

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